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Energies and widths of triply excited states of lithiumlike oxygen and neon

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Abstract. Seven low-lying triply exited states of lithium-like oxygen and neon are calculated with the multichannel saddle-point and saddle-point complex-rotation methods. The term energies are given for these excited states, along with level shifts and partial Auger widths from dominant decay channels. The mass polarization effect and relativistic corrections are included. The radiative transition rates are also calculated. These results are compared with other theoretical data in the literature.

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1 Introduction

The advances of the synchrotron sources and detection techniques have stimulated the considerable experimental and theoretical interests in the study of hollow lithium-like atom, with both $1s$-shell orbitals vacant. It offers an ideal system for investigating the four-body Coulombic problems and for testing the effectiveness of the most advanced theoretical methods in dealing with such problems.

The triply excited $2l^2 2l'$ resonances in lithium were first observed in beam-foil experiments by Bruch *et al.* [1,2]. Triply excited lithium had also been seen by Müller *et al.* [3], Agentoft *et al.* [4], and Mannervik *et al.* [5]. Kiernan *et al.* [6] had measured the resonance energy of lithium $2s^2 2p\ ^2P^0$ using a laser plasma technique. To our knowledge, this is first reported experimental Auger lifetime of a lithium triply excited state. Knystautas *et al.* [7] and Träbert *et al.* [8] had observed the $2P^3\ ^4S^0$ in He$^-$, Be^{2+}, and C^{3+} by its radiative decay. Recently, Kiernan *et al.* [9], Azuma *et al.* [10], and Journel *et al.* [11] had reported the observation of many higher-lying $^2P^0$ resonances using different experimental techniques. The Hartree-Fock configuration interaction method, the multiconfiguration Dirac-Fock method, and the R-matrix method had been carried out to identificate these resonances in these work, respectively. Diehl *et al.* [12] made a high-precision measurement for the energy and width of $2s^2 2p\ ^2P^0$ using the Advanced Light Source facility at Berkeley. Their results 142.28(3) and 0.118(3) eV agree excellently with the prediction of Chung and Gou [13] at 142.255 and 0.1175 eV, respectively. Cubaynes *et al.* [14] made high-precision measurements for energies and widths of $2s2p^2\ ^2P$ and $2s2p^2\ ^2D$ also. Their data 145.08(5) and 0.047(5) eV agree quite well with the prediction of reference [13] at 145.075 and 0.048 eV. This suggests that the saddle-point complex-rotation method [13] is an effective method for autoionizing systems.

Among the earlier theoretical work, Ahmed and lipsky [15] calculated the triply excited resonances of the lithium-like system with a configuration interaction method. Chung *et al.* calculated the triply excited resonances of Li [16] and Be$^+$ [17] using the saddle-point method. The results from the saddle-point method are used to identify the Auger spectra of Li and Be$^+$ observed by Rødbro *et al.* [2]. The calculations of energies and widths of the triply excited resonances are very challenging because there are strong electron correlation effects and an infinite number of open channels associated with these resonances. In Chung and Gou [13,18–20], the saddle-point complex-rotation method is used to calculate the energies and widths of the triply excited Li, Be$^+$, and C^{3+} resonances. Recently, Piangos and Nicolaides [21] calculated the radiative lifetimes of triply excited states of the Li isoelectronic sequence, using the state-specific theory method. To our knowledge, no any high-resolution Auger spectra data and Auger partial width calculation are available for the triply excited O^{5+} and Ne^{7+} in the literature. The reliable theoretical energy data and the partial width information in this work should be useful in the understanding of the experimental spectra for these systems in future.

In this work, seven triply excited states of lithium-like O^{5+} and Ne^{7+} are studied. The resonance positions and widths are calculated with multichannel saddle-point complex-rotation method. A restricted variation method is used to saturate wavefunction space. Relativistic corrections are computed with first-order perturbation theory.

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2 Theory

The non-relativistic Hamiltonian for the upper bound is given in atomic units by

$$H=\sum_{i=1}^{3}\left(-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right)+\sum_{\substack{i,\,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}\cdot \tag{1}$$

In general, the saddle-point wave function of core excited three-electron system [17] can be written as

$$\begin{aligned}\Psi_b=A\sum C_{mnk}^{l_1l_2L_{12}l_3}[1-P(r_1)][1-P(r_2)][1-P(r_3)]\\ \times\phi_{mnk}(r_1,r_2,r_3)Y_{l_1l_2L_{12}}^{l_3LM}(\hat r_1,\hat r_2,\hat r_3)X(1,2,3)\end{aligned} \tag{2}$$

where A is the antisymmetrization operator, the radial basis functions are slater orbitals

$$\phi_{mnk}(r_1,r_2,r_3)=r_1^m r_2^n r_3^k e^{-(\alpha_i r_1+\beta_i r_2+\gamma_i r_3)}. \tag{3}$$

In equation (2) the projection operator is given by

$$P(r_i)=|\phi_0(r)\rangle\langle\phi_0(r)| \tag{4}$$

where the vacancy orbital is

$$\phi_0(r)=N\exp(-qr). \tag{5}$$

The autoionizing states of hollow atomic systems can be thought of as inner shell vacancy states that are quasi-bound. These states are degenerate with the continuum, if the continuum is not carefully removed from the variational wavefunction, in some case this could lead to variational break down. Using saddle-point variational method, q in equation (5) is a parameter determined in the energy maximization processes. The linear parameters C and the nonlinear parameters α_i, β_i, γ_i in equations (2, 3) are determined in the energy optimization processes, we gain the basic wave function Ψ_b and the corresponding saddle-point energy E_b. To further improve energy, we then expend the total wave function as

$$\Psi(1,2,3)=D_0\Psi_b(1,2,3)+\Psi_2(1,2,3) \tag{6}$$

where

$$\Psi_2(1,2,3)=A\sum_{i=1}^{I}D_i\Psi_{n(i),l(i)}(1,2,3). \tag{7}$$

Ψ_2 is a function to saturate the functional space. It takes the same form as $\Psi_b(1,\,2,\,3)$, but the nonlinear parameters are much different from that of $\Psi_b(1,\,2,\,3)$. In practice, we will break up Ψ_2 into many parts. A secular equation will be constructed for each part. Each of the nonlinear parameters in the basis function of Ψ_2 is optimized in the restricted variational calculation [22]. To obtain the width and shift using the saddle-point complex-rotation method [16], we write the total wave function as

$$\Psi(1,2,3)=\Psi_b(1,2,3)+\sum_i A\phi_i(1,2)U_i(3) \tag{8}$$

where

$$U_i=\sum_n d_{i,n}r^n\exp(-\alpha_i r). \tag{9}$$

$\phi_i(1,\,2)$'s are the target states of the open channels. U_i represents the wave function of the outgoing electron. The proper angular and spin coupling between ϕ_i and U_i to obtain the correct total L and M is implicitly assumed in the above equation. When the complex rotation is carried out, we rotate Ψ_b and ϕ_i with the Hamiltonian. The nonlinear parameters obtained from the saddle-point calculation in $\Psi_b(1,\,2,\,3)$ are retained, but the linear parameters are recalculated to allow for full interaction between the closed-channel and the open-channel wave functions. The complex energy obtained from $\Psi(1,\,2,\,3)$, $E-i\Gamma/2$, gives the position and the width of the resonance. The difference, $E_s=E-E_b$, represents the shift from the saddle-point energy to the resonance energy, due to the interaction between $\Psi_b(1,\,2,\,3)$ and the continua. The total nonrelativistic energy is obtained by adding the improvement from restricted variation, ΔE_{RV}, the shift E_s, and the energy upper bound E_b.

The total energy is further improved by including the mass polarization effects and relativistic corrections. The relativistic perturbation operators considered in this work are: correction to the kinetic energy (P^4), the Darwin term, the electron-electron contact term and the orbit-orbit interaction. The explicit expressions of these perturbation operators are given in reference [16], they will not be repeated here.

3 Result and discussion

The seven triply excited O^{5+} and Ne^{7+} systems studied in this work are $2s^22p\ ^2P^0$, $2s2p^2\ ^4P$, $2s2p^2\ ^2D$, $2s2p^2\ ^2S$, $2s2p^2\ ^2P$, $2p^3\ ^2D^0$, and $2p^3\ ^2P^0$, which have been observed [2] and identified [13,19] in Li, Be^+. The nonrelativistic energies of these states are given in Table 1. In this work, all the singly-excited states of O^{6+} or Ne^{8+} are open channels and need to be removed from the saddle-point wavefunctions. The optimized value of q for all these states is close to 8 for oxygen and 10 for neon, since all three electrons are excited to at least the $n=2$ level where their ability to screen the nuclear charge seen by the $1s$ vacancy orbital is small. The triply excited states include strongly degenerate configurations, one must take to include all relevant angular and spin couplings to account for correlations. As Table 1 shows, the number of angular-spin components in the wave function arranges from 17 to 52. To improve the energy obtained from Ψ_b, we use the restricted variational method to compute energy contributions from each chosen angular series. By summing these contributions, these energies are further improved by the restricted variation method with ΔE_{RV} ranges from -36.1 to -147.8 μa.u.

The width and the shift of the resonances are calculated in two steps. First, a partial width is computed with

Table 1. Nonrelativistic energies (in μa.u.) of some low-lying triply excited states of lithium-like oxygen and neon. q is the nonlinear parameter in the vacancy orbitals, N_L is the number of angular-spin components in the wavefunction, N is the number of linear parameters in the basic wavefunction. The widths are given in meV.

Resonances	q	N_L	N	E_b	ΔE_{RV}	E_s	E_{nonrel}	Width
O^{5+}								
$2s2s2p\ ^2P^0$	7.868	38	801	−20733587.2	−123.9	1844.6	−20731866.5	195.02
$2s2p2p\ ^4P$	7.816	18	487	−20718765.9	−40.8	872.7	−20717934.0	17.19
$2s2p2p\ ^2D$	7.864	46	897	−20392262.9	−95.9	2361.7	−20389997.1	198.89
$2s2p2p\ ^2S$	7.872	49	995	−20163139.9	−130.9	3477.7	−20159793.1	123.38
$2s2p2p\ ^2P$	7.972	45	976	−20127242.8	−109.3	−355.8	−20127707.9	129.39
$2p2p2p\ ^2D^0$	7.471	47	964	−20092534.5	−101.8	2015.2	−20090621.1	229.72
$2p2p2p\ ^2P^0$	8.153	48	995	−19838352.4	−109.9	3033.0	−19835429.3	124.61
Ne^{7+}								
$2s2s2p\ ^2P^0$	9.861	48	946	−33374184.1	−147.8	2417.7	−33371914.2	222.65
$2s2p2p\ ^4P$	9.816	19	461	−33359712.4	−36.1	870.3	−33358878.2	18.71
$2s2p2p\ ^2D$	9.864	46	936	−32933502.9	−115.4	1819.8	−32931798.5	250.70
$2s2p2p\ ^2S$	9.867	49	949	−32640363.9	−142.1	3670.5	−32636835.5	120.10
$2s2p2p\ ^2P$	9.970	45	952	−32593727.0	−105.3	−479.0	−32594311.3	137.44
$2p2p2p\ ^2D^0$	9.480	44	903	−32545957.4	−134.4	2453.3	−32543638.5	256.55
$2p2p2p\ ^2P^0$	10.09	40	882	−32218507.1	−69.9	3536.5	−32215040.5	133.05

Table 2. Relativistic energies of some low-lying triply excited resonances of lithium-like oxygen and neon. Here H_1 is the mass polarization, H_2 the P^4 and the Darwin term, the electron-electron contact term, and the orbit-orbit interaction in μa.u. T is the term energy above the $1s^22s$ ground state in eV.

		Perturbation corr.		E_{total}	This work	PN[a]
Resonances	E_{nonrel}	$\langle H_1\rangle$	$\langle H_2\rangle$	(μa.u.)	T	T
O^{5+}						
$2s2s2p\ ^2P^0$	−20731866	4.1	−17283	−20749145	1184.39	1184.53
$2s2p2p\ ^4P$	−20717934	10.4	−13263	−20731187	1184.88	
$2s2p2p\ ^2D$	−20389997	6.9	−13130	−20403120	1193.80	1194.10
$2s2p2p\ ^2S$	−20159793	21.7	−12760	−20172531	1200.08	1200.41
$2s2p2p\ ^2P$	−20127708	14.4	−12580	−20140274	1200.96	1201.43
$2p2p2p\ ^2D^0$	−20090621	16.8	−9014	−20099618	1202.06	1202.35
$2p2p2p\ ^2P^0$	−19835429	27.1	−9524	−19844926	1208.99	1209.44
Ne^{7+}						
$2s2s2p\ ^2P^0$	−33371914	4.4	−41443	−33413353	1888.19	1888.29
$2s2p2p\ ^4P$	−33358878	11.0	−33793	−33392492	1888.75	
$2s2p2p\ ^2D$	−32931799	7.5	−33531	−32965335	1900.38	1900.70
$2s2p2p\ ^2S$	−32636836	23.2	−32748	−32668897	1908.44	1908.74
$2s2p2p\ ^2P$	−32594311	14.9	−32436	−32626732	1909.59	1910.07
$2p2p2p\ ^2D^0$	−32543639	18.0	−23232	−32566888	1911.22	1911.51
$2p2p2p\ ^2P^0$	−32215040	29.4	−24752	−32239763	1920.12	1920.53

[a] Piangos and Nicolaides [21] and relativistic effects are included.

Table 3. Partial widths ($\mathit{\Gamma}_p$) and shifts ($\mathit{\Delta}E_s$), fully coupled width ($\mathit{\Gamma}$) and shift (E_s) of the triply exited states for lithiumlike oxygen ($\mathit{\Gamma}_p$ in meV, $\mathit{\Delta}E_s$ in μa.u.).

	Autoionizing channels								Fully coupled
Resonances	$1s1s\ ^1S$	$1s2s\ ^3S$	$1s2s\ ^1S$	$1s2p\ ^3P$	$1s2p\ ^1P$	$1s3p\ ^3P$	$1s3p\ ^1P$		
				$\mathit{\Gamma}_p$				$\mathit{\Sigma}\mathit{\Gamma}_p$	$\mathit{\Gamma}$
$2s2s2p\ ^2P^0$	14.45	13.73	2.73	122.81	38.79	0.00	0.02	192.53	195.02
$2s2p2p\ ^4P$				17.17		0.01		17.17	17.19
$2s2p2p\ ^2D$	16.34	117.21	2.87	59.19	0.17	0.01	0.00	195.79	198.89
$2s2p2p\ ^2S$	6.74	52.90	0.62	57.46	0.07	0.06	0.00	117.85	123.38
$2s2p2p\ ^2P$				77.48	51.64	0.00	0.01	129.13	129.39
$2p2p2p\ ^2D^0$				171.20	57.19	0.12	0.00	228.51	229.72
$2p2p2p\ ^2P^0$	1.68	1.44	0.25	91.36	30.10	0.21	0.01	125.05	124.61
				$\mathit{\Delta}E_s$				$\mathit{\Sigma}\mathit{\Delta}E_s$	E_s
$2s2s2p\ ^2P^0$	453.80	142.06	162.41	849.01	677.10	116.15	3.18	2403.71	1844.64
$2s2p2p\ ^4P$				872.34		186.10		1058.44	872.69
$2s2p2p\ ^2D$	246.90	1565.00	65.60	260.48	146.59	135.83	4.31	2424.71	2361.70
$2s2p2p\ ^2S$	1077.40	2521.70	2340.00	195.30	168.00	134.50	1.86	6438.76	3477.70
$2s2p2p\ ^2P$				−563.62	281.03	41.99	11.15	−229.45	−355.77
$2p2p2p\ ^2D^0$				1545.40	484.60	−0.78	0.07	2029.29	2015.20
$2p2p2p\ ^2P^0$	123.30	54.00	582.20	3506.40	1199.10	19.39	0.43	4384.82	3033.02

Table 4. Partial widths ($\mathit{\Gamma}_p$) and shifts ($\mathit{\Delta}E_s$), fully coupled width ($\mathit{\Gamma}$) and shift (E_s) of the triply excited states for lithiumlike neon ($\mathit{\Gamma}_p$ in meV, $\mathit{\Delta}E_s$ in μa.u.).

	Autoionizing channels								Fully coupled
Resonances	$1s1s\ ^1S$	$1s2s\ ^3S$	$1s2s\ ^1S$	$1s2p\ ^3P$	$1s2p\ ^1P$	$1s3p\ ^3P$	$1s3p\ ^1P$		
				$\mathit{\Gamma}_p$				$\mathit{\Sigma}\mathit{\Gamma}_p$	$\mathit{\Gamma}$
$2s2s2p\ ^2P^0$	0.43	3.39	39.32	127.23	41.53	0.00	0.01	212.45	222.65
$2s2p2p\ ^4P$				18.94		0.00		18.94	18.71
$2s2p2p\ ^2D$	0.40	130.60	45.30	60.63	0.25	0.01	0.00	247.19	250.70
$2s2p2p\ ^2S$	0.61	38.20	18.40	57.50	0.14	0.04	0.00	114.89	120.10
$2s2p2p\ ^2P$				80.23	56.62	0.00	0.01	136.85	137.44
$2p2p2p\ ^2D^0$				187.73	63.41	0.08	0.00	251.22	256.55
$2p2p2p\ ^2P^0$	0.05	0.43	4.16	94.43	33.13	0.14	0.00	132.34	133.05
				$\mathit{\Delta}E_s$				$\mathit{\Sigma}\mathit{\Delta}E_s$	E_s
$2s2s2p\ ^2P^0$	541.01	220.39	679.30	891.34	760.59	123.74	4.02	3220.39	2417.67
$2s2p2p\ ^4P$				842.40		196.00		1038.40	870.32
$2s2p2p\ ^2D$	17.25	772.40	552.40	179.32	136.40	144.00	5.57	1807.34	1819.83
$2s2p2p\ ^2S$	334.40	1624.40	1955.20	112.50	160.40	144.20	3.03	4334.13	3670.49
$2s2p2p\ ^2P$				−621.27	301.78	45.05	15.15	−259.29	−479.02
$2p2p2p\ ^2D^0$				1820.00	598.51	−0.55	0.07	2418.03	2453.30
$2p2p2p\ ^2P^0$	628.26	51.47	91.09	2402.60	1388.93	18.58	0.38	4581.31	3536.52

Table 5. Transition rate in s^{-1} of some low-lying triply excited resonances of lithium-like oxygen and neon. The number in brackets indicates the powers of 10.

	O^{5+}			Ne^{7+}		
Transition	R_V	R_A	$R_V(\text{PN})^a$	R_V	R_A	$R_V(\text{PN})^a$
$1s^22s\ ^2S \rightarrow 2s^22p\ ^2P^0$	1.44 [9]	8.55 [8]	3.1 [9]	2.41 [9]	1.36 [9]	5.2 [9]
$\rightarrow 2p^3\ ^2P^0$	2.19 [8]	1.15 [8]	1.7 [8]	2.42 [8]	1.40 [8]	2.9 [8]
$1s^22p\ ^2P^0 \rightarrow 2s2p^2\ ^2D$	2.69 [9]	1.41 [9]	3.8 [9]	4.53 [9]	2.32 [9]	6.5 [9]
$\rightarrow 2s2p^2\ ^2P$	7.54 [9]	3.92 [9]	1.1 [10]	1.25 [10]	6.45 [9]	1.9 [10]
$\rightarrow 2s2p^2\ ^2S$	2.48 [9]	1.42 [9]	3.4 [9]	4.15 [9]	2.32 [9]	6.4 [9]
$1s2s^2\ ^2S \rightarrow 2s^22p\ ^2P^0$	1.98 [12]	1.97 [12]	2.0 [12]	5.18 [12]	5.18 [12]	5.1 [12]
$\rightarrow 2p^3\ ^2P^0$	1.70 [10]	1.60 [10]	2.5 [10]	4.18 [10]	3.94 [10]	5.6 [10]
$1s2p^2\ ^2S \rightarrow 2s^22p\ ^2P^0$	2.71 [9]	2.56 [9]	4.2 [9]	8.33 [10]	8.82 [10]	9.6 [9]
$\rightarrow 2p^3\ ^2P^0$	1.43 [12]	1.45 [12]	1.4 [12]	3.68 [12]	3.75 [12]	3.6 [12]
$1s2p^2\ ^2P \rightarrow 2s^22p\ ^2P^0$	3.33 [11]	3.41 [11]	3.7 [11]	8.84 [11]	9.06 [11]	9.4 [11]
$\rightarrow 2p^3\ ^2D^0$	2.98 [12]	3.03 [12]	3.0 [12]	7.70 [12]	7.80 [12]	7.8 [12]
$\rightarrow 2p^3\ ^2P^0$	2.65 [12]	2.62 [12]	2.6 [12]	6.85 [12]	6.77 [12]	6.7 [12]
$1s2p^2\ ^2D \rightarrow 2s^22p\ ^2P^0$	1.92 [11]	1.93 [11]	2.1 [11]	5.06 [11]	5.12 [11]	5.3 [11]
$\rightarrow 2p^3\ ^2D^0$	3.07 [12]	3.09 [12]	3.1 [12]	7.87 [12]	7.90 [12]	7.8 [12]
$\rightarrow 2p^3\ ^2P^0$	1.52 [12]	1.49 [12]	1.5 [12]	3.90 [12]	3.82 [12]	3.8 [12]
$[1s(2s2p)^3P]^2P^0 \rightarrow 2s2p^2\ ^2S$	3.76 [12]	3.66 [12]	3.7 [12]	9.60 [12]	9.38 [12]	9.6 [12]
$\rightarrow 2s2p^2\ ^2P$	4.29 [11]	4.42 [11]	3.5 [11]	1.07 [12]	1.09 [12]	9.1 [11]
$\rightarrow 2s2p^2\ ^2D$	3.70 [12]	3.75 [12]	3.7 [12]	9.47 [12]	9.57 [12]	9.6 [12]
$[1s(2s2p)^1P]^2P^0 \rightarrow 2s2p^2\ ^2S$	4.20 [9]	3.66 [9]		9.20 [12]	9.00 [12]	
$\rightarrow 2s2p^2\ ^2P$	4.15 [8]	3.56 [8]		1.51 [12]	1.55 [12]	
$\rightarrow 2s2p^2\ ^2D$	6.34 [9]	7.63 [9]		9.08 [12]	9.19 [12]	
$1s2s2p^4P^0 \rightarrow 2s2p^2\ ^4P$	4.18 [12]	4.15 [12]		1.06 [13]	1.06 [13]	

[a] Piangos and Nicolaides [21].

only one open channel at a time. We then include all the important open channels in one wavefunction to calculate the total width and the total shift. The energies of the triply excited lithium-like systems lie above the double-ionization threshold, there are an infinite number of open channels in the complex-rotation calculation. The most important contributors to the width of the resonances are open channels associated with the $1s2s\ ^{1,3}S$, $1s2p\ ^{1,3}P$, and $1s3p\ ^{1,3}P$ target states. In this work, some coupled calculations include up to ten open channels. The convergence of the resonances width and shift is checked with respect to the angle of complex scaling (0.3–0.6 rad) and the variation of parameter α_i in equation (9). In many cases, the partial width results are stable to five digits. For all resonances, the sum of the partial widths agrees remarkable well with the total width calculation, the differences are about 4.5% or less. However, the sum of the individual shift may differ substantially with the total shift. These suggests that one may not be able to estimate the full shift from the individual shifts. In the total nonrelativistic term energy calculation we have included the shift from the fully coupled calculation.

In addition to the shift E_s and ΔE_{RV}, the energy of the resonances is further corrected by the mass polarization and relativistic perturbations. The mass polarization perturbation operator is accurate to all orders. The relativistic corrections are calculated using first-order perturbation theory. We note that the mass polarization corrections vary smoothly as a function of nuclear charge. Using the $1s^22s$ ground-state energy $O^{5+}_{rel} = -64.2760837$, and $Ne^{7+}_{rel} = -102.8048003$ a.u. [23], the term energy of these resonances can be calculated. These results are given in Table 2. For all cases, the term energies are lower than these of Piangos and Nicolaides [21]. In this table, the energies from reference [21] are corrected with relativistic corrections.

In Tables 3 and 4, we reported the partial widths and shifts, fully coupled width and shift of the triply excited states for lithium-like oxygen and neon. The target states considered in this work are $1s^2\ ^1S$, $1s2s\ ^{1,3}S$, $1s2p\ ^{1,3}P$, and $1s3p\ ^{1,3}P$, others such as $1snl$ $(n \geq 4)$ are neglected. The number of open channels depends on the symmetry of the resonances. For $2s^22p\ ^2P^0$, there are six major channels: $1s2s\ ^{1,3}S + kp$, $1s2p\ ^{1,3}P + ks$, and $1s2p\ ^{1,3}P + kd$, whereas for $2s2p^2\ ^4P$ there is only one major open channel.

Table 6. Width (Γ_A), radiative rate (W_R), Auger transition rate (W_A), Auger branching ratio (η_A), and lifetime (τ) of some low-lying triply excited states of lithium-like oxygen and neon.

Resonances	Γ_A (meV)	W_R (10^{13} s^{-1})	W_A (10^{13} s^{-1})	η_A (%)	τ (10^{-15} s)
O^{5+}					
$2s2s2p\ ^2P^0$	195	0.25	29.63	99.2	3.3
$2s2p2p\ ^4P$	17	0.42	2.58	86.0	33.3
$2s2p2p\ ^2D$	199	0.37	30.23	98.8	3.3
$2s2p2p\ ^2S$	123	0.38	18.69	98.0	5.2
$2s2p2p\ ^2P$	129	0.04	19.60	99.8	5.1
$2p2p2p\ ^2D^0$	230	0.61	34.94	98.3	2.8
$2p2p2p\ ^2P^0$	125	0.56	18.99	97.1	5.1
Ne^{7+}					
$2s2s2p\ ^2P^0$	223	0.66	33.88	98.1	2.9
$2s2p2p\ ^4P$	19	1.06	2.89	73.2	25.3
$2s2p2p\ ^2D$	251	1.86	38.13	95.3	2.5
$2s2p2p\ ^2S$	120	1.88	18.23	90.7	5.0
$2s2p2p\ ^2P$	137	0.26	20.81	98.8	4.7
$2p2p2p\ ^2D^0$	257	1.56	39.05	96.2	2.5
$2p2p2p\ ^2P^0$	133	1.45	20.21	93.3	4.6

Therefore for $2s2p^2\ ^4P$ states of O^{5+} (or Ne^{7+}) the width is 17.19 meV (18.71 meV) much less than 195.02 meV (222.65 meV) of $2s^22p\ ^2P^0$ state. In the Tables 3 and 4, the $1s2s\ ^{1,3}S$ and $1s2p\ ^{1,3}P$ channels have most large contributors to the width of the resonances (*via* the $1/r_{ij}$ interrelation repulsion perturbation), since in this case the initial- and final-states have more approximate electron configurations. In general, the shift E_s is positive, for a few states it is negative and small. The small shifts shown in the table seem to justify the inner shell vacancy picture. Note that the sum of the individual shift may differ substantially with the total shift, but the sum of the partial width agree with remarkable well with the total width calculation. We are not aware of any high-resolution Auger spectra data for the triply excited O^{5+} and Ne^{7+} available. The theoretical data in this work should be useful for studying these Auger spectra in future experiments.

Table 5 gives the computed optical transition rates from the dipole-velocity (R_V) and dipole-acceleration (R_A) formulae. The results include one-photon-one-electron transition to one-photon-three-electron transition. The results for one-photon-three-electron transition are not expected to be highly accurate because these oscillator strengths are calculated with Ψ_b only. The open channel part of the wavefunction is not included. Nevertheless, the R_V with R_A in this work give reasonable agreement with the data of Piangos and Nicolaides [21]. In Table 6, the results show that the optical emission rates are very small in comparison with the Auger decay rates of the triply excited states for systems considered in this work. The lifetimes of the triply excited states of lithium-like oxygen and neon are about 10^{-14}–10^{-15} s.

4 Conclusion

In this work, we have made a detailed atomic structure and spectra study on the seven triply excited states of lithium-like oxygen and neon. For each state, the results for the upper bound, the nonrelativistic energy, the partial widths, the shift, the term energy, the transition rates, and the lifetime are reported. We have used a restricted-variation method for the nonrelativistic energy and a multichannel saddle-point complex-rotation method for the shift and width. Excellent convergence is found in this calculation. The relativistic corrections and the mass polarization effects are included. For all cases, the term energies are lower than the previously published values. These data for O^{5+} and Ne^{7+} should be very useful in future experiments.

We have also calculated the radiative transition rates for the triply excited resonances. Our conclusion is that radiative transition rates are extremely small to compare with the corresponding Auger rates. For radiative rates in this work the dipole-velocity and dipole-acceleration formulae results agree reasonably well. For a few rates which are relatively small, the two results do not agree closely because we have not included the effect of the open channel in these calculations. We have not investigated the higher resonances of each symmetry in this work, but the method used here should be applicable for these higher resonances.

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